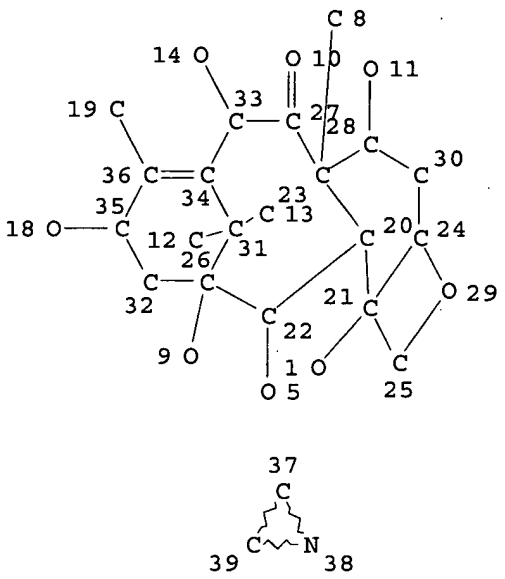
=> d 12
L2 HAS NO ANSWERS
L2 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE

=> s l2 ful
FULL SEARCH INITIATED 08:26:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 9661 TO ITERATE

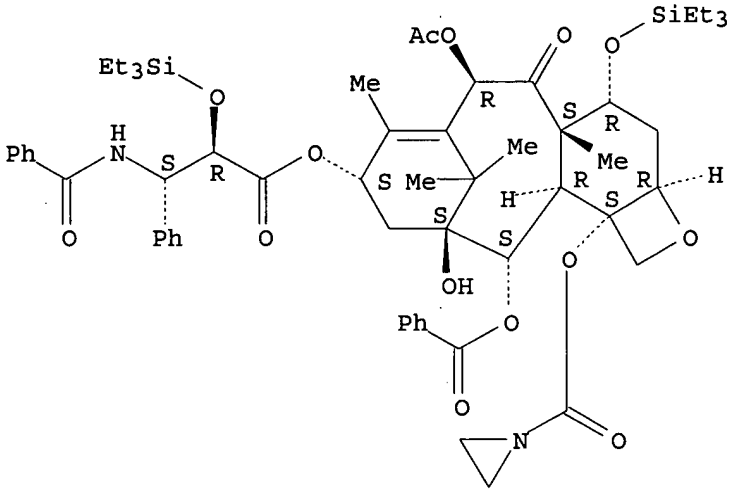
100.0% PROCESSED 9661 ITERATIONS 8 ANSWERS
SEARCH TIME: 00.00.01

L4 8 SEA SSS FUL L2

=> d 1-8

L4 ANSWER 1 OF 8 REGISTRY COPYRIGHT 2005 ACS on STN
RN 165883-72-7 REGISTRY
ED Entered STN: 08 Aug 1995
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-9-[3-(benzoylamino)-1-oxo-3-phenyl-2-[(triethylsilyl)oxy]propoxy]-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4α,4aβ,6β,9α(2R*,3S*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C60 H80 N2 O14 Si2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

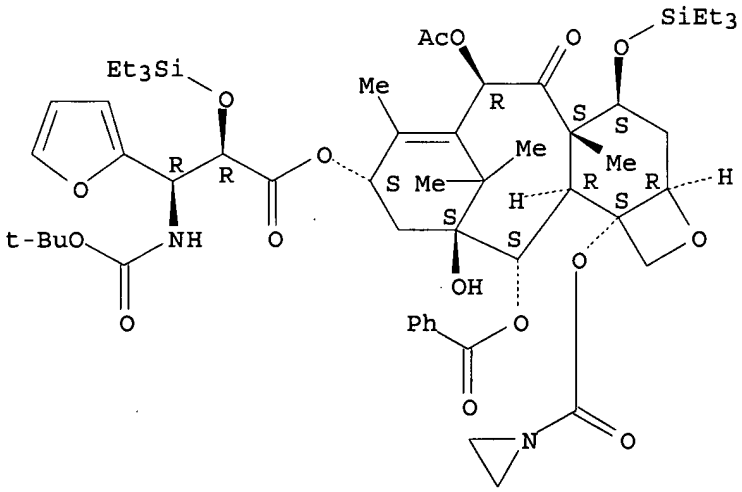
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 2 OF 8 REGISTRY COPYRIGHT 2005 ACS on STN
RN 165686-31-7 REGISTRY
ED Entered STN: 03 Aug 1995
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-12-(benzoyloxy)-9-[3-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(2-furanyl)-1-oxo-2-[(triethylsilyl)oxy]propoxy]-3,4,4a,5,6,9,10,11,12,12a-decahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(2R*,3R*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C56 H82 N2 O16 Si2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

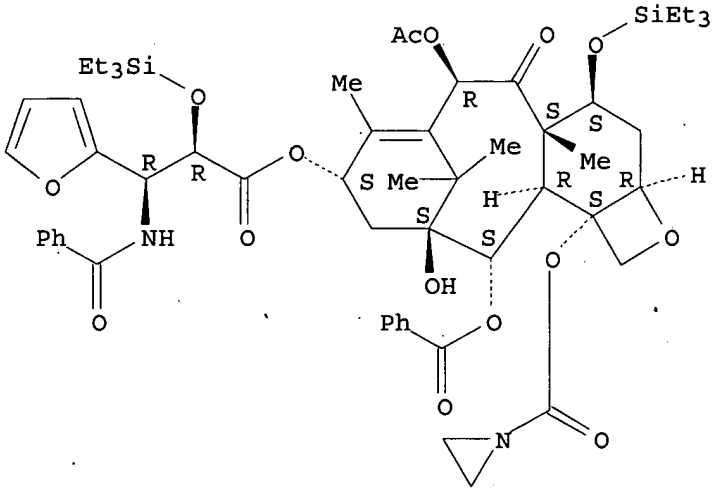
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 3 OF 8 REGISTRY COPYRIGHT 2005 ACS on STN
RN 165686-30-6 REGISTRY
ED Entered STN: 03 Aug 1995
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-9-[3-(benzoylamino)-1-oxo-3-(2-furanyl)-2-[(triethylsilyl)oxy]propoxy]-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(2R*,3R*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C58 H78 N2 O15 Si2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

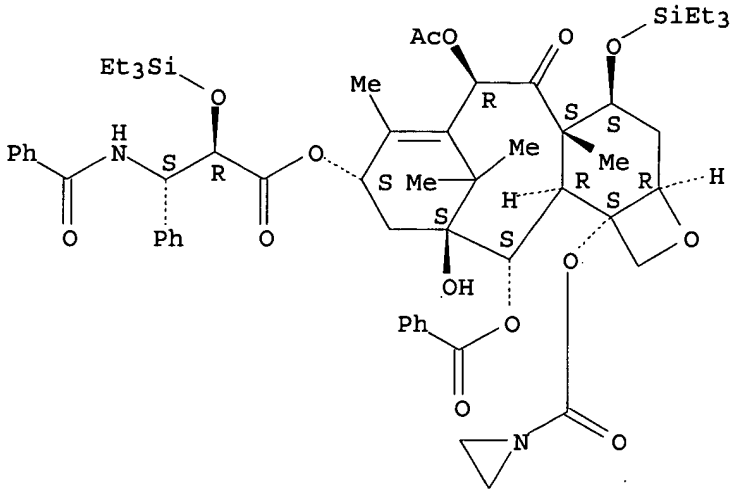
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 4 OF 8 REGISTRY COPYRIGHT 2005 ACS on STN
RN 165686-29-3 REGISTRY
ED Entered STN: 03 Aug 1995
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-9-[3-(benzoylamino)-1-oxo-3-phenyl-2-[(triethylsilyl)oxy]propoxy]-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(2R*,3S*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C60 H80 N2 O14 Si2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

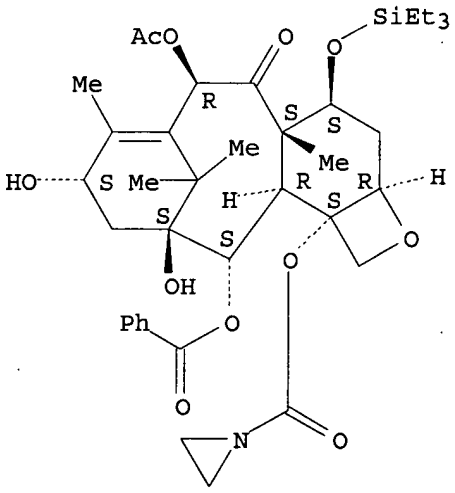
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 5 OF 8 REGISTRY COPYRIGHT 2005 ACS on STN
RN 165686-28-2 REGISTRY
ED Entered STN: 03 Aug 1995
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-9,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-(2aα,4β,4aβ,6β,9α,11.alpha.,12α,12aα,12bα)]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C38 H53 N O11 Si
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



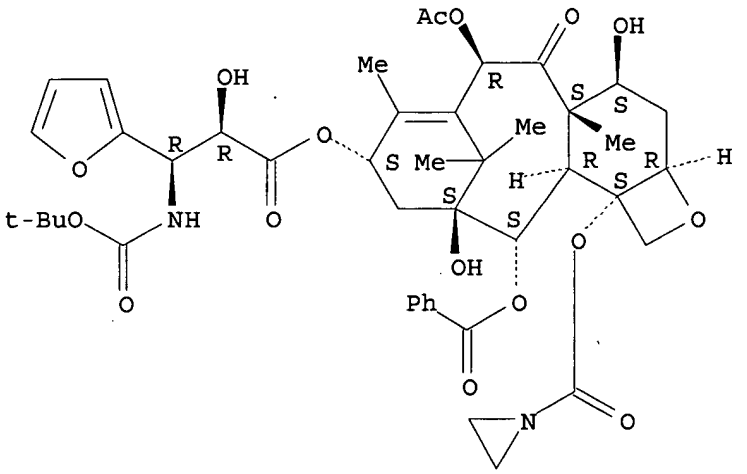
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 6 OF 8 REGISTRY COPYRIGHT 2005 ACS on STN
RN 165686-23-7 REGISTRY
ED Entered STN: 03 Aug 1995
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-12-(benzoyloxy)-9-[3-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(2-furanyl)-2-hydroxy-1-oxopropoxy]-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(2R*,3R*),11α,12.alpha.,12aα,12bα]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C44 H54 N2 O16
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

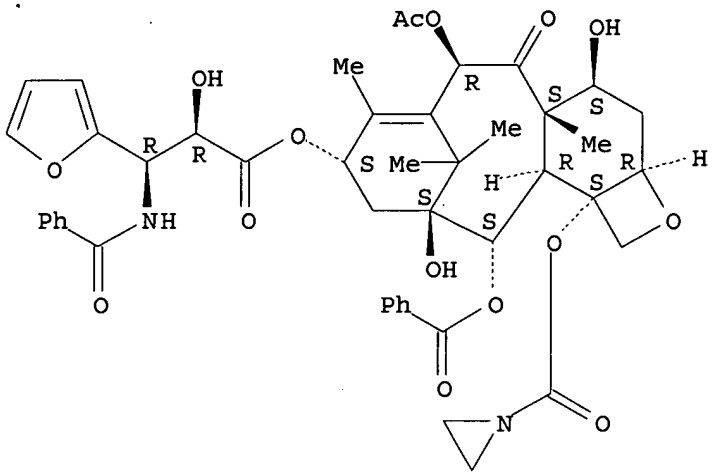
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 7 OF 8 REGISTRY COPYRIGHT 2005 ACS on STN
RN 165686-22-6 REGISTRY
ED Entered STN: 03 Aug 1995
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-9-[3-(benzoylamino)-3-(2-furanyl)-2-hydroxy-1-oxopropoxy]-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(2R*,3R*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C46 H50 N2 O15
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

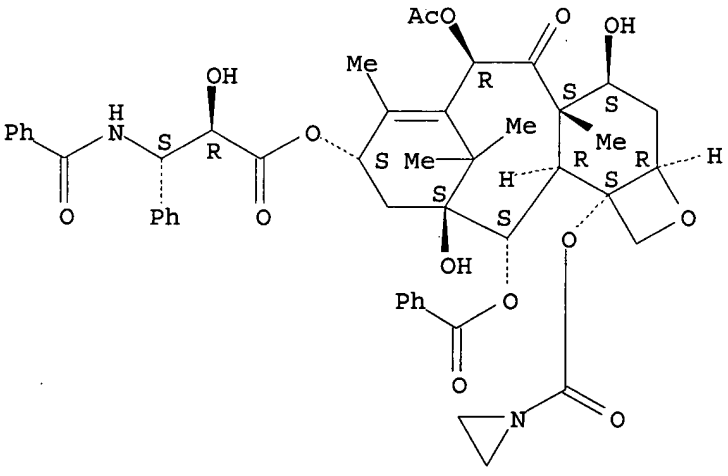
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

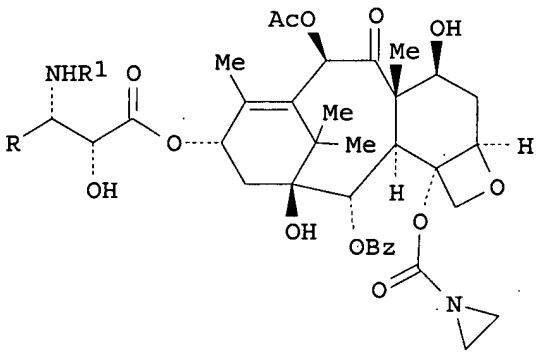
L4 ANSWER 8 OF 8 REGISTRY COPYRIGHT 2005 ACS on STN
RN 165686-21-5 REGISTRY
ED Entered STN: 03 Aug 1995
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-9-[3-(benzoylamino)-2-hydroxy-1-oxo-3-phenylpropoxy]-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(2R*,3S*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C48 H52 N2 O14
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

AN 1995:591877 CAPLUS
DN 123:112445
TI Synthesis and Biological Evaluation of Novel C-4 Aziridine-Bearing Paclitaxel (Taxol) Analogs
AU Chen, Shu-Hui; Fairchild, Craig; Long, Byron H.
CS Bristol-Myers Squibb Pharmaceutical Research Institute, Wallingford, CT, 06492-7660, USA
SO Journal of Medicinal Chemistry (1995), 38(12), 2263-7
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI



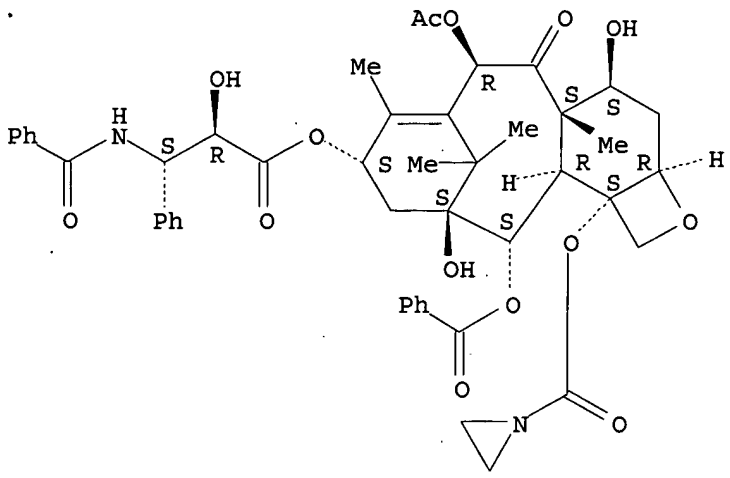
I

AB Three novel C-4 aziridine-bearing paclitaxel analogs I (R = 2-furyl, Ph; R1 = Bz, Boc) were synthesized during the course of our continuing effort at C-4 modification. The key step in the synthesis is the aziridine ring formation at the C-4 position via an intramol. Mitsunobu reaction. The syntheses and the biol. evaluation of these C-4 aziridine-containing derivs. are herein discussed.

IT **165686-21-5P 165686-22-6P 165686-23-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of novel C-4 aziridine-bearing paclitaxel (taxol) analogs)

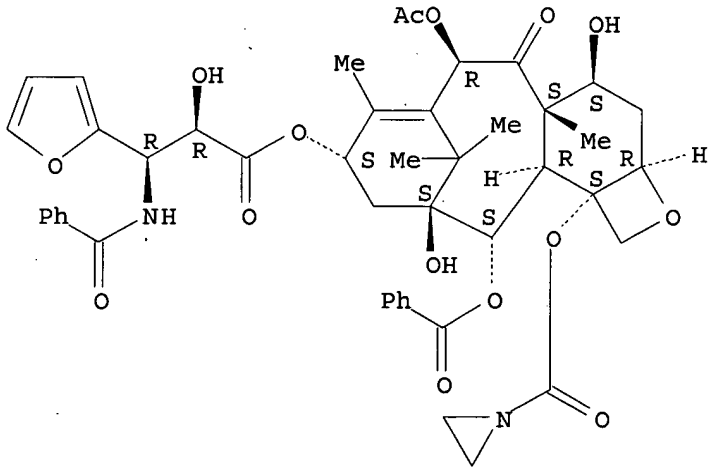
RN 165686-21-5 CAPLUS
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-9-[3-(benzoylamino)-2-hydroxy-1-oxo-3-phenylpropoxy]-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(2R*,3S*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



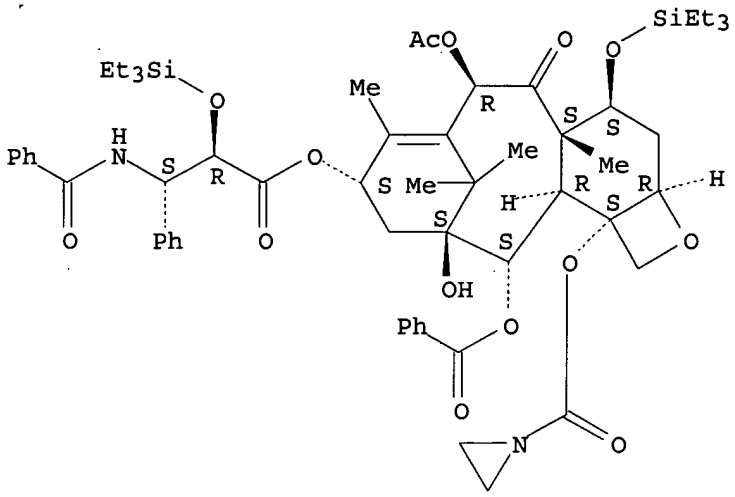
RN 165686-22-6 CAPLUS
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-9-[3-(benzoylamino)-3-(2-furanyl)-2-hydroxy-1-oxopropoxy]-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(2R*,3R*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



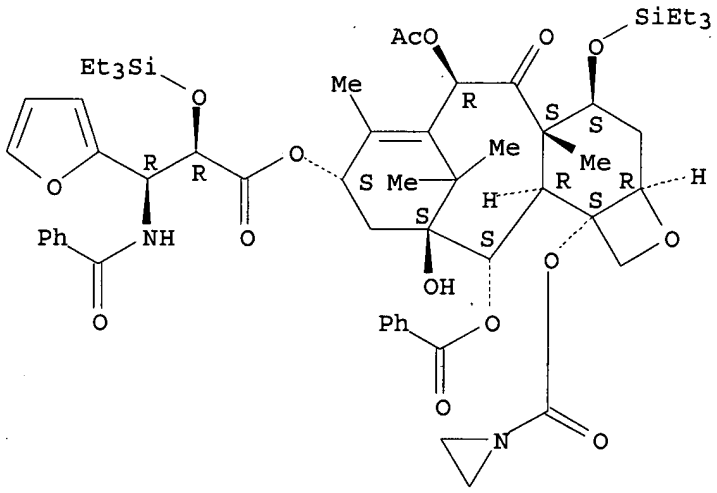
RN 165686-23-7 CAPLUS
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-12-(benzoyloxy)-9-[3-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(2-furanyl)-2-hydroxy-1-oxopropoxy]-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(2R*,3R*),11α,12.alpha.,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



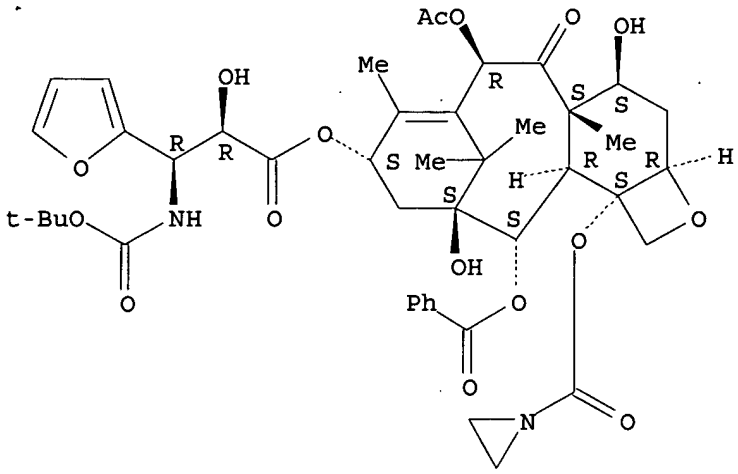
RN 165686-30-6 CAPLUS
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-9-[3-(benzoylamino)-1-oxo-3-(2-furanyl)-2-[(triethylsilyl)oxy]propoxy]-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(2R*,3R*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 165686-31-7 CAPLUS
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-12-(benzoyloxy)-9-[3-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(2-furanyl)-1-oxo-2-[(triethylsilyl)oxy]propoxy]-3,4,4a,5,6,9,10,11,12,12a-decahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(2R*,3R*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

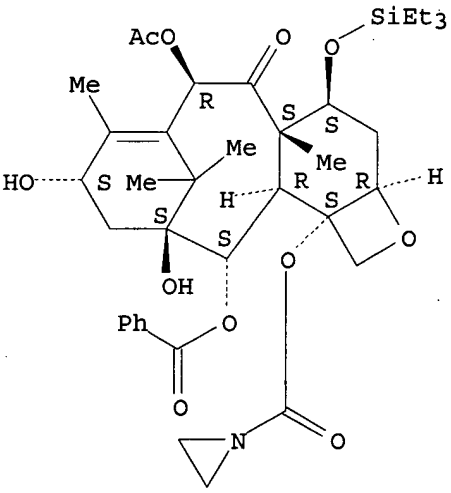


IT **165686-28-2P 165686-29-3P 165686-30-6P**
165686-31-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. evaluation of novel C-4 aziridine-bearing paclitaxel (taxol) analogs)

RN 165686-28-2 CAPLUS

CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-9,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-(2aα,4β,4aβ,6β,9α,11.alpha.,12α,12aα,12bα)]- (9CI) (CA INDEX NAME)

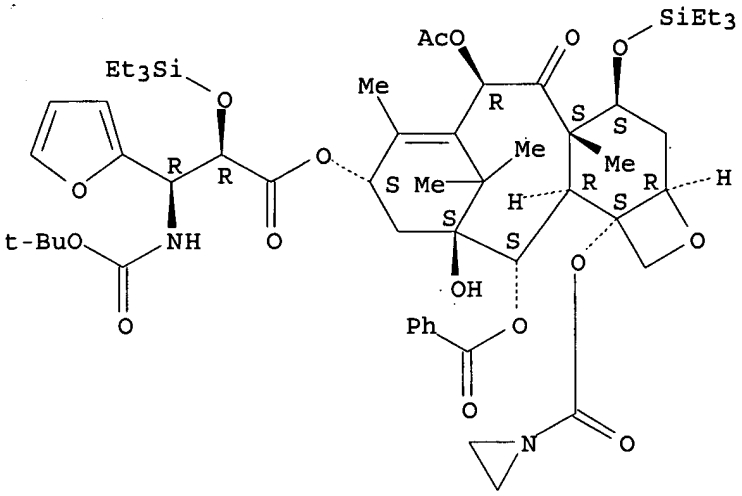
Absolute stereochemistry.



RN 165686-29-3 CAPLUS

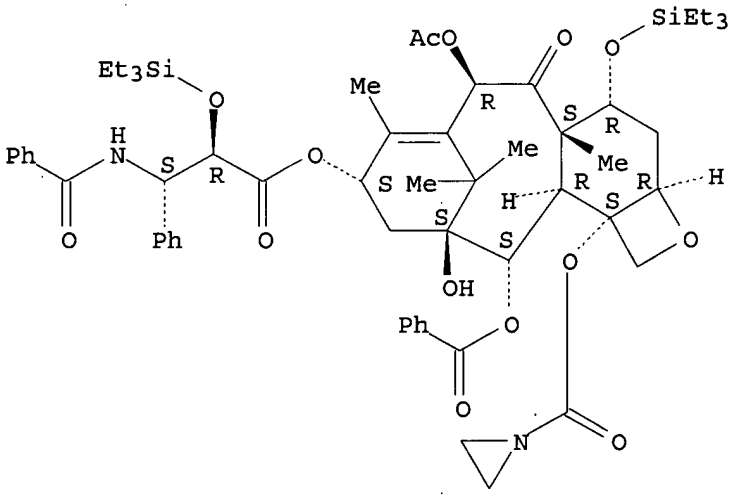
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-9-[3-(benzoylamino)-1-oxo-3-phenyl-2-[(triethylsilyl)oxy]propoxy]-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(2R*,3S*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **165883-72-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and biol. evaluation of novel C-4 aziridine-bearing paclitaxel (taxol) analogs)
RN 165883-72-7 CAPLUS
CN 1-Aziridinecarboxylic acid, 6-(acetyloxy)-9-[3-(benzoylamino)-1-oxo-3-phenyl-2-[(triethylsilyl)oxy]propoxy]-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-[(triethylsilyl)oxy]-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl ester, [2aR-[2aα,4α,4aβ,6β,9α(2R*,3S*),11α,12α,12aα,12bα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L2 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:700179 CAPLUS
DN 130:37942
TI Computer-assisted design and synthetic applications of chiral enol borinates: novel, highly enantioselective aldol reagents
AU Gennari, Cesare; Ceccarelli, Simona; Piarulli, Umberto; Aboutayab, Karim
CS Dipartimento di Chimica Organica e Industriale, Centro CNR per lo Studio delle Sostanze Organiche Naturali, Universita di Milano, Milan, I-20133, Italy
SO Journal of the Brazilian Chemical Society (1998), 9(4), 319-326
CODEN: JOCSET; ISSN: 0103-5053
PB Sociedade Brasileira de Quimica
DT Journal; General Review
LA English
AB A review with >16 refs. We have recently described the development of a quant. transition state model for the prediction of stereoselectivity in the boron-mediated aldol reaction. This model provides qual. insights into the factors contributing to the stereochem. outcome of a variety of reactions of synthetic importance. The force field model was used to assist the design and preparation of new chiral boron ligands derived from menthone. The chiral boron enolates were employed in various stereoselective processes, including the addition to chiral aldehydes and the reagent-controlled total synthesis of (3S,4S)-statine. The chiral enolates derived from α-halo and α-oxy-substituted thioacetates were added to aldehydes and imines. Addition to imines leads to the enantioselective synthesis of chiral **aziridines**, a formal total synthesis of (+)-thiamphenicol, and a new highly efficient synthesis of the paclitaxel (taxol) C-13 side-chain and taxol semisynthesis from **baccatin** III. The stereochem. outcome of the addition to imines was rationalized with the aid of computational studies. Enantioselective addition reactions of the chiral boron enolate derived from thioacetate have successfully been applied to solid phase bound aldehydes to give aldol products in comparable yields and enantioselectivities to the usual solution conditions.
RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT
AB A review with >16 refs. We have recently described the development of a quant. transition state model for the prediction of stereoselectivity in the boron-mediated aldol reaction. This model provides qual. insights into the factors contributing to the stereochem. outcome of a variety of reactions of synthetic importance. The force field model was used to assist the design and preparation of new chiral boron ligands derived from menthone. The chiral boron enolates were employed in various stereoselective processes, including the addition to chiral aldehydes and the reagent-controlled total synthesis of (3S,4S)-statine. The chiral enolates derived from α-halo and α-oxy-substituted thioacetates were added to aldehydes and imines. Addition to imines leads to the enantioselective synthesis of chiral **aziridines**, a formal total synthesis of (+)-thiamphenicol, and a new highly efficient synthesis of the paclitaxel (taxol) C-13 side-chain and taxol semisynthesis from **baccatin** III. The stereochem. outcome of the addition to imines was rationalized with the aid of computational studies. Enantioselective addition reactions of the chiral boron enolate derived from thioacetate have successfully been applied to solid phase bound aldehydes to give aldol products in comparable yields and enantioselectivities to the usual solution conditions.

L2 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:219135 CAPLUS
DN 126:293369
TI Rationally designed chiral enol borinates: powerful reagents for the stereoselective synthesis of natural products
AU Gennari, C.

CS Dip. Chim. Org. Ind., Univ. Milano, Milan, 20133, Italy
SO Pure and Applied Chemistry (1997), 69(3), 507-512
CODEN: PACHAS; ISSN: 0033-4545
PB Blackwell
DT Journal; General Review
LA English
AB A review, with .apprx.15 refs. The authors recently described the development of a quant. transition state model for the prediction of stereoselectivity in the B-mediated aldol reaction. This model provides qual. insights into the factors contributing to the stereochem. outcome of a variety of reactions of synthetic importance. The force field model was used to assist the design and preparation of new chiral B ligands derived from menthone. The chiral B enolates were used in various stereoselective processes, including the addition to chiral aldehydes and the reagent-controlled total synthesis of (3S,4S)-statine. The chiral enolates derived from α-halo and α-oxysubstituted thioacetates were added to aldehydes and imines. Addition to imines leads to the enantioselective synthesis of chiral **aziridines**, a formal total synthesis of (+)-thiamphenicol, and a new highly efficient synthesis of the paclitaxel (taxol®) C-13 side-chain and taxol semisynthesis from **baccatin** III. The stereochem. outcome of the addition to imines was rationalized with the aid of computational studies.
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT
AB A review, with .apprx.15 refs. The authors recently described the development of a quant. transition state model for the prediction of stereoselectivity in the B-mediated aldol reaction. This model provides qual. insights into the factors contributing to the stereochem. outcome of a variety of reactions of synthetic importance. The force field model was used to assist the design and preparation of new chiral B ligands derived from menthone. The chiral B enolates were used in various stereoselective processes, including the addition to chiral aldehydes and the reagent-controlled total synthesis of (3S,4S)-statine. The chiral enolates derived from α-halo and α-oxysubstituted thioacetates were added to aldehydes and imines. Addition to imines leads to the enantioselective synthesis of chiral **aziridines**, a formal total synthesis of (+)-thiamphenicol, and a new highly efficient synthesis of the paclitaxel (taxol®) C-13 side-chain and taxol semisynthesis from **baccatin** III. The stereochem. outcome of the addition to imines was rationalized with the aid of computational studies.
ST review chiral enol borinate reagent; natural product stereoselective synthesis borinate review; force field design enol borinate review; statine synthesis enol borinate reagent review; **aziridine** chiral synthesis enol borinate review; thiamphenicol formal synthesis enol borinate review; paclitaxel synthesis enol borinate reagent review; taxol semisynthesis **baccatin** III borinate review; menthone boron deriv reagent review